On the fine structure photodetachment intensities using the irreducible tensorial expression of second quantization operators

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Abstract. The fine-structure relative intensities of photodetachment in S^- at the vicinity of the threshold have been calculated recently [1] to analyze the microscope photodetachment images produced by the s-photoelectron. The branching ratios were obtained using the electric dipole approximation and the standard irreducible tensorial operator techniques. The same authors observed that these relative intensities were consistent with the Cox-Engelking-Lineberger formula [2] derived from the fractional parentage approach [3], in which the laser photon annihilates one of the p-electrons of the negative ion to promote it into the s-continuum. This agreement between the two formalisms was qualified as *remarkable*.

With this paper, we show that this agreement is understood from a *general* interesting angular momentum expression relating a weighted sum of squared $9j$-symbols and a weighted sum of products of squared $6j$-symbols. We point out that the "standard" approach result is a special case of Pan and Starace's parametrization [5] of the photodetachment cross sections in the term-independent approximation. The link with the Cox-Engelking-Lineberger result established in their work makes the agreement between the standard and the fractional parentage methods even more natural. The present work provides another elegant and deep link between the two formalisms thanks to the irreducible tensorial expression of the second quantization form of the electric dipole transition operator. Indeed, the $(SL)J$-coupled form of the latter reproduces Pan and Starace's cross section expression from which the standard result can be derived, while the $9j$-coefficient characterizing the fractional parentage Cox-Engelking-Lineberger formula quickly emerges when using its $(jj)J$ coupling form.

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1. Introduction

The fine structure of S and S$^-$ have been measured recently using the photodetachment microscope technique [1]. In the Appendix of that work, branching ratios of the fine structure components for s-wave photodetachment of ^{32}S$^-$ were calculated using a "standard" approach and compared with the results deduced from the "fractional parentage" formula of Engelking and Lineberger [2] based on Cox's treatment [4, 3]. As resumed in section 2, the two formalisms yield the same numerical results. A similar agreement between the two approaches, that appears as a "surprise" at first sight of the rather different expressions, was found in the study of the relative intensities of the hyperfine components of photodetachment from ^{17}O$^-$ [6]. We show how the two formulae can be related to each other through an interesting general angular momentum algebra relation that is proven in the Appendix using a graphical approach. In their analysis, the authors of both publications [6, 1] made no mention of the important work of Pan and Starace [5]. Yet, the latter does integrate the "standard" approach formula in the case of photodetachment of a p-subshell electron for which limiting the partial waves summation to the lowest value ($l = 0$) according to Wigner's threshold law [7], leads to a complete separation of dynamical and geometric factors. Moreover, a link between their general expression of the partial photoionization cross section and the previously published results [3, 2, 8, 9, 10] was already established in [5]. Since Pan and Starace's contribution escaped to the attention of authors of recent publications on photodetachment and since the mention of the link with the Cox-Engelking-Lineberger results was limited in [5] to a rather short statement accompanied by a brief footnote, it is worthwhile to investigate Blondel *et al*'s "surprise" adopting Pan and Starace's point of view. This is done in section 3. In section 4, we first show how the Pan and Starace's cross section expression can be derived adopting the irreducible tensorial expression of the second quantization form of the electric dipole transition operator. We then show that the $9j$-coefficient, characterizing the fractional parentage Cox-Engelking-Lineberger formula, emerges naturally from the recoupling of the annihilation and creation operators, from $(SL)J$ to $(jj)J$ coupling.

2. A "surprising" agreement

The photodetachment process from a single open-shell anion is written as

$$\text{X}^-[n_i l_i^N \ (S_i L_i) J_i] \ + \ (\hbar\omega) \rightarrow \text{X}[n_i l_i^{N-1} \ (S_a L_a) J_a] \ + \ e^-[(s l_c) j_c] \tag{1}$$

where the i, a and c indices refer to the negative *i*on, the neutral *a*tom and the *c*ontinuum electron, respectively.

2.1. The "standard" approach

Assuming pure LS coupling and using the Wigner law [7] in the vicinity of the photodetachment threshold for setting the quantum numbers of the ejected electron ($l_c = 0, j_c = s = 1/2$), Blondel *et al* [1] derived the relative intensities of the fine structure components for the detachment of a *p*-electron from the "standard" Wigner-Racah algebra [11, 12] in the electric dipole approximation :

$$\mathcal{I}(J_a, J_i) = \sum_J [\, J_a, J_i, J\,] \begin{Bmatrix} L_a & J & S_i \\ s & S_a & J_a \end{Bmatrix}^2 \begin{Bmatrix} J & 1 & J_i \\ L_i & S_i & L_a \end{Bmatrix}^2 \tag{2}$$

with the abbreviated notation

$$[j_1, j_2, \ldots] \equiv (2j_1 + 1)(2j_2 + 1) \ldots$$

2.2. The fractional parentage formula

Describing the photodetachment as a direct one-electron process in which the laser photon "annihilates" an electron of angular momentum l_i to promote it into the continuum, the relative intensities can be calculated from the formula of Engelking and Lineberger [2]

$$\mathcal{I}(J_a, J_i) = \sum_{j_i} [\, J_a, J_i, j_i\,] \begin{Bmatrix} S_a & L_a & J_a \\ s & l_i & j_i \\ S_i & L_i & J_i \end{Bmatrix}^2, \tag{3}$$

using the fractional parentage approach of Cox [4, 3]. Expression (3) is hereafter referred to as the "Cox-Engelking-Lineberger" fractional parentage formula.

2.3. The S^-/S relative branching ratios of the fine-structure thresholds

The relative branching ratios of the fine-structure thresholds for the *s*-wave photodetachment of ^{32}S$^-$

$$\text{S}^- \, [3p^5 \, ^2P^o_{J_i}] \;+\; (\hbar\omega) \rightarrow \text{S} \, [3p^4 \, ^3P_{J_a}] \;+\; e^-[(l_c = 0; j_c = 1/2)]. \tag{4}$$

are reported in Table 1, according to Blondel *et al* [1]. As observed by these authors, the two formalisms based on equations (2) and (3) yield identical results. A similar agreement between the two approaches, that was presented as a "surprise" at first sight of the rather different expressions, was found in the study of the hyperfine structure relative intensities of photodetachment of ^{17}O$^-$ [6].

2.4. An interesting angular momentum algebra relation

The agreement between the numerical results obtained from equations (2) and (3) is not limited to the above quantum number values and can not be accidental. We found,

Table 1. Relative branching ratios of the fine-structure thresholds.

$J_i(S^-)$	$J_a(S)$	$\mathcal{I}(J_a, J_i)$
1/2	0	4/54
	1	9/54
	2	5/54
3/2	0	2/54
	1	9/54
	2	25/54

using a graphical approach [13, 14, 15] presented in Appendix A, an interesting *general* angular momentum relation

$$\sum_j [j] \begin{Bmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j \\ j_6 & j_7 & j_8 \end{Bmatrix}^2 = \sum_{j'} [j'] \begin{Bmatrix} j_2 & j_6 & j' \\ j_4 & j_3 & j_1 \end{Bmatrix}^2 \begin{Bmatrix} j_2 & j_6 & j' \\ j_8 & j_5 & j_7 \end{Bmatrix}^2, \tag{5}$$

that, as shown in Appendix, is a special case of equation (33)/sect.12.2 of Varshalovich *al.* [15].

Applied in our context, relation (5) gives

$$\sum_\alpha [\alpha] \begin{Bmatrix} S_a & L_a & J_a \\ s & l_i & \alpha \\ S_i & L_i & J_i \end{Bmatrix}^2 = \sum_\beta [\beta] \begin{Bmatrix} L_a & \beta & S_i \\ s & S_a & J_a \end{Bmatrix}^2 \begin{Bmatrix} \beta & l_i & J_i \\ L_i & S_i & L_a \end{Bmatrix}^2. \tag{6}$$

To the knowledge of the authors, relation (5) cannot be found as such in the current literature.

The link between (6) with the "standard" and fractional parentage formulae is established as follows:

(i) In the l.h.s of (6), α plays the role in the fractional parentage formalism (equation (3)) of the possible j-values of the extracted electron in the negative ion, ie. $\alpha = j_i = l_i \pm 1/2$.

(ii) In the r.h.s of (6), β plays the role in the standard approach (equation (2)) of the total angular momentum J of the composite system (neutral atom + electron), ie. $\beta = (J_a s)J = (J_a j_c)J$.

Note that the entry "1" in the middle of the upper line of the second $6j$-symbol of the standard formula (2) corresponds to the rank one of the electric dipole (E1) transition

operator. It appears in our relation (6) as the angular momentum value of the shell loosing one electron in the photodetachment process, restricting the above analysis to the photodetachment from a p-shell. However, this restriction is not too serious since this is precisely what Blondel *et al* [1] needed in their "standard" approach for generating the s-outgoing electron wave as the dominant channel from Wigner's threshold law.

3. Pan and Starace's analysis

Pan and Starace [5] parametrized the relative photoionization and photodetachment cross sections for fine structure transitions, starting from

$$\sigma(J_a, J_i) = \frac{4\pi^2\omega}{c[J_i]} \sum_{M_i M l_c j_c J} | \, \hat{\boldsymbol{\epsilon}} \cdot \langle \, (S_a L_a) J_a, (s l_c) j_c, JM- | \mathbf{D} | (S_i L_i) J_i M_i \, \rangle \, |^2, \tag{7}$$

where $\mathbf{D} \equiv \sum_{k=1}^{N} \mathbf{r}_k$ is the electric dipole operator and $\hat{\boldsymbol{\epsilon}}$ is the polarization vector of the incident light of frequency ω. The minus sign appearing in the bra indicates that the final state wave functions satisfy incoming-wave boundary conditions [16]. The final state of the composite system (neutral atom + electron) is characterized by the total angular momentum J using the $(J_a j_c)J$ coupling, where $(s l_c)j_c$ results from the coupling of the spin $(s = 1/2)$ and the outgoing partial wave associated to the continuum photoelectron. For the photodetachment process (1), they got the following *general* result‡

$$\sigma(J_a, J_i) = \frac{4\pi^2\omega}{3c} \, [J_a, S_i, L_i, l_i] \, N \, (\, S_a L_a, l_i \, |\} \, S_i L_i \,)^2 \tag{8}$$

$$\times \sum_{l_c} [l_c] \sum_L \sum_{L'} [L, L'] \begin{pmatrix} l_c & 1 & l_i \\ 0 & 0 & 0 \end{pmatrix}^2 (\, \epsilon l_c \, | \, r \, | \, n_i l_i \,)_L (\, \epsilon l_c \, | \, r \, | \, n_i l_i \,)_{L'} \exp i (\phi_{\epsilon l_c}^L - \phi_{\epsilon l_c}^{L'})$$

$$\times \begin{Bmatrix} l_c & l_i & 1 \\ L_i & L & L_a \end{Bmatrix} \begin{Bmatrix} l_c & l_i & 1 \\ L_i & L' & L_a \end{Bmatrix} \begin{bmatrix} L_a & S_a & S_i & L_i & L \\ & J_a & 1/2 & J_i & 1 & l_c \\ L_a & S_a & S_i & L_i & L' \end{bmatrix},$$

where $(\, \epsilon l_c \, | \, r \, | \, n_i l_i \,)_L$ is the one-electron radial E1 matrix element depending on the LS quantum numbers of the transition, $\phi_{\epsilon l_c}^L$ is the phase shift of the photoelectron with respect to a plane wave [16] and L (L') appears as the angular momentum of the composite system [neutral atom (L_a) + electron (l_c)]. The last symbol with the 15 entries is a $15j$-symbol of the second kind [18, 15].

3.1. The "standard" formula: a special case of (8)

Considering the case of the photodetachment of an open p-subshell electron and setting $l_c = 0$ according to Wigner's threshold law, allows for a complete separation of dynamical and geometric factors and reduces (8) to:

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‡ We observed that the square of the $3j$-symbol is missing in (7) of Pan and Starace [5]. This has been confirmed by Starace [17].

$$\sigma_{l=0}(J_a, J_i) = \frac{4\pi^2\omega}{3c}[J_a, S_i, L_i] \, N \, (p^{N-1} \, S_aL_a, p \,|\} \, p^N S_i L_i \,)^2$$

$$\times \, (\, \epsilon s \,|\, r \,|\, n_i l_i \,)^2_{L=L_a} \delta_{l_i,1} \sum_J [\, J\,] \begin{Bmatrix} L_a & S_i & J \\ s & J_a & S_a \end{Bmatrix}^2 \begin{Bmatrix} L_a & S_i & J \\ J_i & 1 & L_i \end{Bmatrix}^2. \tag{9}$$

In this expression, one recognizes the summation over the product of the two squared $6j$-symbols appearing in the standard approach formula (2). As pointed out in the introduction, the fact that Pan and Starace's analysis [5] integrated this result as a special case of (8), escaped to the attention of the authors of publications [1] and [6].

3.2. The term-independent approximation

Pan and Starace [5] have also shown that, if the radial matrix elements are assumed independent of the angular momenta L and L' (the so-called *term-independent* (TI) approximation), the partial photoionization cross section (8) reduces to

$$\sigma^{TI}(J_a, J_i) = \frac{4\pi^2\omega}{3c} \sum_{l_c} [l_c] \begin{pmatrix} l_c & 1 & l_i \\ 0 & 0 & 0 \end{pmatrix}^2 (\, \epsilon l_c \,|\, r \,|\, n_i l_i \,)^2 \, [J_a, S_i, L_i] \tag{10}$$

$$\times \, N \, (\, S_aL_a, l_i \,|\} \, S_i L_i \,)^2 \, \sum_J [\, J\,] \begin{Bmatrix} L_a & S_i & J \\ s & J_a & S_a \end{Bmatrix}^2 \begin{Bmatrix} L_a & S_i & J \\ J_i & 1 & L_i \end{Bmatrix}^2.$$

3.3. Linking Pan and Starace TI cross section with previous works

Pan and Starace [5] were linking the partial photodetachment cross section derived in the term-independent approximation with all previous results [3, 2, 8, 9, 10] through the following short statement:

"*Equation (10)§ is equivalent to the single-configuration, LS-coupling, term-independent results of others*",

referring to a brief footnote commenting the existence of some relations between "*the sum over a squared $9j$-coefficient and an alternative way of representing the same $12j$-coefficient that we represent as a sum over a product of squared $6j$-coefficients*".

The relation behind this footnote is nothing else than the angular momentum algebra relation (5) demonstrated in Appendix A.

§ numbered as (13) in the original reference [5].

4. Using the irreducible tensorial expression of second quantization operators

Using the spherical components of the photon polarization vector and of the electric dipole moment, the scalar product appearing in (7) is written as [19]

$$\hat{\boldsymbol{\epsilon}} \cdot \mathbf{D} = \sum_{q=-1}^{+1} \epsilon_{-q}^{(1)} D_q^{(1)} = \sum_{q=-1}^{+1} \epsilon_q^{(1)*} D_q^{(1)} \,. \tag{11}$$

Applying the Wigner-Eckart theorem and using the $3j$-symbol orthogonality, one easily finds [20]

$$\sum_{M_i M} |\,\hat{\boldsymbol{\epsilon}} \cdot \langle\, \gamma J M - |\, \mathbf{D} \,|\, \gamma_i J_i M_i \,\rangle\,|^2 = \frac{1}{3}|\, \langle\, \gamma J - ||\, D^{(1)} \,||\, \gamma_i J_i \,\rangle\,|^2 \,, \tag{12}$$

where the minus sign in the bra indicates that we refer to the wave function satisfying the incoming-wave boundary conditions [16]. The partial cross section (7) then reduces to

$$\sigma(J_a, J_i) = \frac{4\pi^2 \omega}{3c[J_i]} \sum_{l_c} \mathcal{D}^{l_c}(J_a, J_i) \,, \tag{13}$$

with

$$\mathcal{D}^{l_c}(J_a, J_i) \equiv \sum_{j_c J} |\, \langle\, (S_a L_a) J_a, (s, l_c) j_c, J - ||\, D^{(1)} \,||\, (S_i L_i) J_i \,\rangle\,|^2 \,. \tag{14}$$

4.1. Second quantized form of transition operators

In the second quantization formalism [21, 22], any one-body operator $F = \sum_i f_i$ takes the form

$$F = \sum_{\xi,\eta} a_\xi^\dagger \,\langle \xi | f | \eta \rangle\, a_\eta \,. \tag{15}$$

The creation $a_\sigma^\dagger$ operators, where σ stands for $(nlm_s m_l)$, form the components of a double tensor $\mathbf{a}^{\dagger(sl)}$ of rank s with respect to spin and rank l with respect to orbit [21]. Similarly, a double tensor can be created from the collection of annihilation operators but a phase factor must be introduced [21] for defining the components $\tilde{a}_\sigma$

$$\tilde{a}_{nlm_s m_l} = (-1)^{s+l-m_s-m_l} a_{nl-m_s-m_l}$$

that form the double tensor $\mathbf{a}^{(sl)}$. It becomes then possible to build the coupled tensors [19]

$$\left[\mathbf{a}^{\dagger(sl)} \times \mathbf{a}^{(sl')}\right]_{\pi q}^{(\kappa k)} = \sum_{\xi,\eta} (sm_{s_\xi} sm_{s_\eta} | ss\kappa\pi)(lm_{l_\xi} l'm_{l_\eta} | ll'kq) \, a_\xi^\dagger \tilde{a}_\eta \,. \tag{16}$$

Using the atomic shell theory [23], the second quantized form of the one-electron operator (15) is written in the following $(SL)J$-coupling tensorial form [24]:

$$F = \sum_{n_i l_i, n_j l_j} [K_S, K_L]^{-\frac{1}{2}} (n_i s l_i \| f^{K_S K_L} \| n_j s l_j) \left[\mathbf{a}^{\dagger(sl_i)} \times \mathbf{a}^{(sl_j)}\right]_{M_J}^{(K_S K_L) K_J} \,, \tag{17}$$

where K_S, K_L and K_J specify the rank with respect to spin, orbit and total angular momentum, respectively, and where $(n_i sl_i \| f^{K_S K_L} \| n_j sl_j)$ is the appropriate one-electron reduced matrix element. In the single-configuration picture, one can pick up from this double sum over the active shells the specific term inducing the desired one-electron jump $i \leftarrow j$, ie.

$$\mathbf{T}_{M_J}^{(K_S K_L)K_J}(i \leftarrow j) = [K_S, K_L]^{-\frac{1}{2}}(n_i sl_i \| f^{K_S K_L} \| n_j sl_j)\left[\mathbf{a}^{\dagger(sl_i)} \times \mathbf{a}^{(sl_j)}\right]_{M_J}^{(K_S K_L)K_J} . \tag{18}$$

For the photodetachment process (1) described in the electric dipole approximation, the transition operator appearing in (14) has the tensorial structure $(K_S K_L)K_J = (01)1$ and is written as

$$\mathbf{T}_Q^{(01)1}(\epsilon l_c \leftarrow n_i l_i) = [1]^{-\frac{1}{2}} t(\epsilon sl_c, n_i sl_i) \left[\mathbf{a}^{\dagger(sl_c)} \times \mathbf{a}^{(sl_i)}\right]_Q^{(01)1} \quad ; \quad Q = 0, \pm 1 , \tag{19}$$

where $t(\epsilon sl_c, n_i sl_i)$ stands for the one-electron E1 reduced matrix element

$$t(\epsilon sl_c, n_i sl_i) = \langle \epsilon sl_c \| \mathbf{t}^{(01)} \| n_i sl_i \rangle \equiv \langle \epsilon sl_c \| \mathbf{S}^{(0)} \mathbf{C}^{(1)} r \| n_i sl_i \rangle .$$

As suggested by Pan and Starace [5] and by equation (8), one needs to integrate in its expression a phase factor for the incoming-wave boundary conditions [16], together with an explicit‖ subscript L for discussing a possible term-dependency of the radial matrix element [25]:

$$t_L(\epsilon sl_c, n_i sl_i) = \langle \epsilon sl_c \| \mathbf{t}^{(01)} \| n_i sl_i \rangle_L = \langle \epsilon sl_c \| \mathbf{S}^{(0)} \mathbf{C}^{(1)} r \| n_i sl_i \rangle_L$$

$$= (-1)^{l_c}[s, l_c, l_i]^{\frac{1}{2}} \begin{pmatrix} l_c & 1 & l_i \\ 0 & 0 & 0 \end{pmatrix} (\epsilon l_c \,|\, r \,|\, n_i l_i)_L \exp i(\phi_{\epsilon l_c}^L). \tag{20}$$

4.2. In $(SL)J$-coupling

The $\mathcal{D}^{l_c}(J_a, J_i)$ contribution (14) to the partial cross section (13) is written as

$$\mathcal{D}^{l_c}(J_a, J_i) = \sum_{Jj_c} \left| \langle (S_a L_a)J_a, (sl_c)j_c, J \| \mathbf{T}_{\epsilon l_c \leftarrow n_i l_i}^{(01)1} \| (S_i L_i)J_i \rangle \right|^2 . \tag{21}$$

To evaluate the matrix element, one first recouples the final combined system, transforming the bra from jj- to SL-coupling [19, 26]

$$\langle (S_a L_a)J_a, (sl_c)j_c, J \,| = \sum_{SL} [S, L, J_a, j_c]^{\frac{1}{2}} \begin{Bmatrix} S_a & s & S \\ L_a & l_c & L \\ J_a & j_c & J \end{Bmatrix} \langle (S_a s)S, (L_a l_c)L, J \,| . \tag{22}$$

Using (19) and (22), (21) becomes

$$\mathcal{D}^{l_c}(J_a, J_i) = \sum_{Jj_c} \left| \sum_{SL} t_L(\epsilon sl_c, n_i sl_i)[S, L, J_a, j_c]^{\frac{1}{2}}[1]^{-\frac{1}{2}} \begin{Bmatrix} S_a & s & S \\ L_a & l_c & L \\ J_a & j_c & J \end{Bmatrix} \right.$$

$$\left. \times \langle (S_a s)S, (L_a l_c)L, J \| \left[\mathbf{a}^{\dagger(sl_c)} \times \mathbf{a}^{(sl_i)}\right]^{(01)1} \| (S_i L_i)J_i \rangle \right|^2 . \tag{23}$$

The J-dependency within the reduced matrix element of the $(SL)J$ coupled creation and annihilation tensor product is extracted using

‖ also implicitly containing the quantum numbers S, L_a and S_a.

$$\langle (S_a s)S, (L_a l_c)L, J \, || \, \left[\mathbf{a}^{\dagger (sl_c)} \times \mathbf{a}^{(sl_i)}\right]^{(01)1} || \, (S_i L_i) J_i \rangle \; = \tag{24}$$

$$[J, 1, J_i]^{\frac{1}{2}} \begin{Bmatrix} S & L & J \\ S_i & L_i & J_i \\ 0 & 1 & 1 \end{Bmatrix} \langle (S_a s)S, (L_a l_c)L \, || \, \left[\mathbf{a}^{\dagger (sl_c)} \times \mathbf{a}^{(sl_i)}\right]^{(01)} || \, S_i L_i \rangle \; .$$

Thanks to the zero entry, the $9j$-symbol simplifies to

$$\begin{Bmatrix} S & L & J \\ S_i & L_i & J_i \\ 0 & 1 & 1 \end{Bmatrix} = (-1)^{L_i + J + S_i + 1} [1, S_i]^{-\frac{1}{2}} \begin{Bmatrix} J_i & L_i & S_i \\ L & J & 1 \end{Bmatrix}. \tag{25}$$

After inserting explicitly the empty continuum space into the bra describing the ion state, (23) becomes

$$\mathcal{D}^{l_c}(J_a, J_i) = \sum_{Jj_c} \Bigg| \sum_{SL} t_L(\epsilon s l_c, n_i s l_i)[S, L, J_a, j_c, J, J_i]^{\frac{1}{2}}[1, S_i]^{-\frac{1}{2}}$$

$$\times (-1)^{L_i + J + S_i + 1} \begin{Bmatrix} S_a & s & S \\ L_a & l_c & L \\ J_a & j_c & J \end{Bmatrix} \begin{Bmatrix} J_i & L_i & S_i \\ L & J & 1 \end{Bmatrix}$$

$$\times \langle (S_a s)S, (L_a l_c)L \, || \, \left[\mathbf{a}^{\dagger (sl_c)} \times \mathbf{a}^{(sl_i)}\right]^{(01)} || \, (S_i 0)S_i, (L_i 0)L_i \rangle \; \Bigg|^2. \tag{26}$$

The matrix element of the tensor product of creation and annihilation operators is expressed in terms of submatrix elements involving the individual operators by introducing a summation over a complete set of intermediate states $S'L'$ [19, 26],

$$\mathcal{D}^{l_c}(J_a, J_i) = \sum_{Jj_c} \Bigg| \sum_{SL} t_L(\epsilon s l_c, n_i s l_i)[S, L, J_a, j_c, J, J_i]^{\frac{1}{2}}[1, S_i]^{-\frac{1}{2}}$$

$$\times (-1)^{L_i + J + S_i + 1} \begin{Bmatrix} S_a & s & S \\ L_a & l_c & L \\ J_a & j_c & J \end{Bmatrix} \begin{Bmatrix} J_i & L_i & S_i \\ L & J & 1 \end{Bmatrix}$$

$$\times (-1)^{S + S_i + L + 1}[1]^{\frac{1}{2}} \sum_{S'L'} \begin{Bmatrix} s & s & 0 \\ S_i & S & S' \end{Bmatrix} \begin{Bmatrix} l_c & l_i & 1 \\ L_i & L & L' \end{Bmatrix}$$

$$\times \langle (S_a s)S, (L_a l_c)L \, || \, \mathbf{a}^{\dagger (sl_c)} || \, (S'0)S', (L'0)L' \rangle$$

$$\times \langle (S'0)S', (L'0)L' \, || \, \mathbf{a}^{(sl_i)} || \, (S_i 0)S_i, (L_i 0)L_i \rangle \; \Bigg|^2. \tag{27}$$

The reduction of the $6j$-symbol

$$\begin{Bmatrix} s & s & 0 \\ S_i & S & S' \end{Bmatrix} = \delta(sSS')(-1)^{s + S + S'}[s, S]^{-\frac{1}{2}} \delta(S_i, S) \tag{28}$$

simplifies the summation over S, thanks to the Kronecker delta¶. After realizing that the creation operator acts only on the continuum space, the first reduced matrix element

¶ The $\delta(ijk)$ notation represents $+1$ if the triangle relations are satisfied and 0 otherwise.

appearing in (27) is evaluated by using the uncoupling formula for reduced matrix elements [19, 26]

$$
\langle (S_a s) S, (L_a l_c) L \, || \, \mathbf{a}^{\dagger (s l_c)} \, || \, (S'0) S', (L'0) L' \rangle
$$
$$
= \delta(S_a, S') \delta(L_a, L') (-1)^{S_a + S + s + L_a + L + l_c} [S, S', L, L']^{\frac{1}{2}}
$$
$$
\times \begin{Bmatrix} S_a & s & S \\ s & S' & 0 \end{Bmatrix} \begin{Bmatrix} L_a & l_c & L \\ l_c & L' & 0 \end{Bmatrix} \langle s l_c \, || \, \mathbf{a}^{\dagger (s l_c)} \, || \, 00 \rangle . \tag{29}
$$

Using the reduced matrix element of the creation operator

$$
\langle s l_c \, || \, \mathbf{a}^{\dagger (s l_c)} \, || \, 00 \rangle = -[s, l_c]^{\frac{1}{2}} , \tag{30}
$$

in agreement with the $N = 1$ limit case of Judd's expression [21])

$$
\langle \psi \, || \, \mathbf{a}^{\dagger} \, || \, \overline{\psi} \rangle = (-1)^N \{ N[S, L] \}^{\frac{1}{2}} (\psi \{ | \overline{\psi}) , \tag{31}
$$

(29) becomes

$$
\langle (S_a s) S, (L_a l_c) L \, || \, \mathbf{a}^{\dagger (s l_c)} \, || \, (S'0) S', (L'0) L' \rangle
$$
$$
= -[S, L]^{\frac{1}{2}} \, \delta(S_a s S) \delta(L_a L_c L) \, \delta(S_a, S') \delta(L_a, L') . \tag{32}
$$

The second reduced matrix element appearing in (27) is worked out similarly for the annihilation operator acting in the $n_i l_i$ shell space

$$
\langle (S'0) S', (L'0) L' \, || \, \mathbf{a}^{(s l_i)} \, || \, (S_i 0) S_i, (L_i 0) L_i \rangle
$$
$$
= (-1)^{S' + S_i + s + L' + L_i + l_i} [S', S_i, L', L_i]^{\frac{1}{2}}
$$
$$
\times \begin{Bmatrix} S' & S_i & s \\ S_i & S' & 0 \end{Bmatrix} \begin{Bmatrix} L' & L_i & l_i \\ L_i & L' & 0 \end{Bmatrix} \langle S' L' \, || \, \mathbf{a}^{(s l_i)} \, || \, S_i L_i \rangle . \tag{33}
$$

Using the annihilation operator reduced matrix element (see equation (32) of [21])

$$
\langle S' L' \, || \, \mathbf{a}^{(s l_i)} \, || \, S_i L_i \rangle = \sqrt{N_i} (-1)^{N_i + S' - s - S_i + L' - l_i - L_i}
$$
$$
\times [S_i, L_i]^{\frac{1}{2}} \, (S' L', l_i \, | \} \, S_i L_i) , \tag{34}
$$

(33) becomes

$$
\langle (S'0) S', (L'0) L' \, || \, \mathbf{a}^{(s l_i)} \, || \, (S_i 0) S_i, (L_i 0) L_i \rangle \tag{35}
$$
$$
= \delta(S' S_i s) \delta(L' L_i l_i) \, \sqrt{N_i} (-1)^{N_i + S' - s - S_i + L' - l_i - L_i} \, [S_i, L_i]^{\frac{1}{2}} \, (S' L', l_i \, | \} \, S_i L_i) .
$$

Combining equations (27), (32) and (35), and taking $N_i = N$ according to (1), the summations over S, S' and L' are reduced to give

$$
\mathcal{D}^{l_c}(J_a, J_i) = \sum_{J j_c} \bigg| (-1)^{J + N + S_i + L_a - l_i} \, \sqrt{N/2} \, (S_a L_a, l_i \, | \} \, S_i L_i) \, [J_a, j_c, J, J_i, S_i, L_i]^{\frac{1}{2}}
$$
$$
\times \sum_L t_L(\epsilon s l_c, n_i s l_i) (-1)^L [L]
$$
$$
\times \begin{Bmatrix} S_a & s & S_i \\ L_a & l_c & L \\ J_a & j_c & J \end{Bmatrix} \begin{Bmatrix} J_i & L_i & S_i \\ L & J & 1 \end{Bmatrix} \begin{Bmatrix} l_c & l_i & 1 \\ L_i & L & L_a \end{Bmatrix} \bigg|^2 ,
$$

$$\mathcal{D}^{l_c}(J_a, J_i) = \frac{N}{2} [J_a, J_i, S_i, L_i] |(S_a L_a, l_i |\} S_i L_i)|^2$$

$$\times \sum_{Jj_c} [j_c, J] \sum_{L} \sum_{L'} t_L(\epsilon s l_c, n_i s l_i) t_{L'}^*(\epsilon s l_c, n_i s l_i)(-1)^{L+L'}[L][L']$$

$$\times \begin{Bmatrix} S_a & s & S_i \\ L_a & l_c & L \\ J_a & j_c & J \end{Bmatrix} \begin{Bmatrix} S_a & s & S_i \\ L_a & l_c & L' \\ J_a & j_c & J \end{Bmatrix} \begin{Bmatrix} J_i & L_i & S_i \\ L & J & 1 \end{Bmatrix} \begin{Bmatrix} J_i & L_i & S_i \\ L' & J & 1 \end{Bmatrix}$$

$$\times \begin{Bmatrix} l_c & l_i & 1 \\ L_i & L & L_a \end{Bmatrix} \begin{Bmatrix} l_c & l_i & 1 \\ L_i & L' & L_a \end{Bmatrix}. \tag{36}$$

Using graphical techniques [13, 14, 15, 18], (36) is finally rewritten as

$$\mathcal{D}^{l_c}(J_a, J_i) = \frac{N}{2} [J_a, J_i, S_i, L_i] |(S_a L_a, l_i |\} S_i L_i)|^2 \tag{37}$$

$$\times \sum_{L} \sum_{L'} t_L(\epsilon s l_c, n_i s l_i) t_{L'}^*(\epsilon s l_c, n_i s l_i)[L, L'] \begin{Bmatrix} l_c & l_i & 1 \\ L_i & L & L_a \end{Bmatrix} \begin{Bmatrix} l_c & l_i & 1 \\ L_i & L' & L_a \end{Bmatrix}$$

$$\times \begin{bmatrix} L_a & S_a & S_i & L_i & L & \\ & J_a & 1/2 & J_i & 1 & l_c \\ L_a & S_a & S_i & L_i & L' & \end{bmatrix}.$$

From the definition of the one-electron reduced matrix element (20), the link with section 3 can be done, in particular with Pan and Starace's general parametrization (8), after using (13) for building the partial cross section. In other terms, one has reproduced Pan and Starace's cross section expression (see however the footnote on page 5), adopting the irreducible tensorial expression of the second quantized form of the electric dipole operator. The particular cases of the "standard" and the term-independent cross sections, discussed in section 3 (see equations (9) and (10), respectively), can obviously be derived from this common result.

4.3. In $(jj)J$-coupling

In the previous subsection, the calculation was performed in $(SL)J$-coupling. The annihilation operator acted on the ion and annihilated the electron $|sl_i\rangle$. The creation operator acted on the vacuum and created the photoelectron. This photoelectron was coupled to the outgoing atom to intermediate $|SL\rangle$ states. These states were recoupled to the final $\langle (J_a, j_c)J|$ state. If one applies the term-independent approximation, the summation over the intermediate states leads to the result (8) that is independent of the intermediate states.

In the present section, the term-independent approximation is used from the very beginning. The final state is obviously $(jj)J$-coupled. So is the initial state if the continuum vacuum is added $|(S_i L_i)J_i\rangle = |(S_i L_i)J_i, (00)0, J\rangle$. The summation over intermediate states introduced in $(SJ)L$-coupling (see previous subsection) is not needed if the spin-angular part of the operator, that is the coupled tensorial product of the

creation and annihilation operator appearing in (18), is recoupled from $(K_S K_L) K_J$ to $(jj)J$

$$\mathbf{T}_{M_J}^{(K_S K_L) K_J}(i \leftarrow j) = [K_S, K_L]^{-\frac{1}{2}} (n_i s l_i \| f^{K_S K_L} \| n_j s l_j) \Big[\mathbf{a}^{\dagger (s l_i)} \times \mathbf{a}^{(s l_j)} \Big]_{M_J}^{(K_S K_L) K_J}$$

$$= (n_i s l_i \| f^{K_S K_L} \| n s l_j) \sum_{j_p j_q} [j_p, j_q]^{\frac{1}{2}} \begin{Bmatrix} K_S & K_L & K_J \\ s & l_i & j_p \\ s & l_j & j_q \end{Bmatrix} \Big[\mathbf{a}^{\dagger (s l_i)} \times \mathbf{a}^{(s l_j)} \Big]_{M_J}^{(j_p j_q) K_J}. \qquad (38)$$

The ranks j_p and j_q are used for the creation and annihilation operators, respectively. This transformation is pure angular recoupling, without affecting the one-electron matrix elements. In other words, the $(SL)J - (jj)J$ recoupling is performed without invoking the full-relativistic approach[+]. The one-electron matrix elements are kept as the non-relativistic, term-independent quantities used in the previous section. Setting the ranks to $K_S = 0, K_L = 1$ and $K_J = 1$ for the electric dipole photodetachment process, with $Q = M_J = 0, \pm 1$, the operator (38) has the form

$$\mathbf{T}_Q^{(01)1}(\epsilon l_c \leftarrow n_i l_i) = t(\epsilon s l_c, n_i s l_i) \Big[\mathbf{a}^{\dagger (s l_c)} \times \mathbf{a}^{(s l_i)} \Big]_Q^{(01)1}$$

$$= t(\epsilon s l_c, n_i s l_i) \sum_{j_p j_q} [j_p, j_q]^{\frac{1}{2}} \begin{Bmatrix} 0 & 1 & 1 \\ s & l_c & j_p \\ s & l_i & j_q \end{Bmatrix} \Big[\mathbf{a}^{\dagger (s l_c)} \times \mathbf{a}^{(s l_i)} \Big]_Q^{(j_p j_q) 1}, \qquad (39)$$

where the one-electron reduced matrix elements are the term-independent form of (20):

$$t(\epsilon s l_c, n_i s l_i) = \langle \epsilon s l_c \| \mathbf{t}^{(01)} \| n_i s l_i \rangle = (-1)^{l_c} [s, l_c, l_i]^{\frac{1}{2}} \begin{pmatrix} l_c & 1 & l_i \\ 0 & 0 & 0 \end{pmatrix} (\epsilon l_c \| r \| n_i l_i). \qquad (40)$$

Using the following reduction

$$\begin{Bmatrix} 0 & 1 & 1 \\ s & l_c & j_p \\ s & l_i & j_q \end{Bmatrix} = (-1)^{j_p + l_i + 1 + s} [1, s]^{-\frac{1}{2}} \begin{Bmatrix} j_q & j_p & 1 \\ l_c & l_i & s \end{Bmatrix}, \qquad (41)$$

the transformed electric dipole operator simplifies to

$$\mathbf{T}_Q^{(01)1}(\epsilon l_c \leftarrow n_i l_i) = t(\epsilon s l_c, n_i s l_i) \sum_{j_p j_q} [j_p, j_q]^{\frac{1}{2}} [1, s]^{-\frac{1}{2}} (-1)^{j_p + l_i + 1 + s}$$

$$\times \begin{Bmatrix} j_q & j_p & 1 \\ l_c & l_i & s \end{Bmatrix} \Big[\mathbf{a}^{\dagger (s l_c)} \times \mathbf{a}^{(s l_i)} \Big]_Q^{(j_p j_q) 1}, \qquad (42)$$

that is used for expressing (21) as

$$\mathcal{D}^{l_c}(J_a, J_i) = \sum_{J j_c} \Big| t(\epsilon s l_c, n_i s l_i) \sum_{j_p j_q} [j_p, j_q]^{\frac{1}{2}} [1, s]^{-\frac{1}{2}} (-1)^{j_p + l_i + 1 + s} \begin{Bmatrix} j_q & j_p & 1 \\ l_c & l_i & s \end{Bmatrix}$$

$$\times \langle (S_a L_a) J_a, (s l_c) j_c, J \| \Big[\mathbf{a}^{\dagger (s l_c)} \times \mathbf{a}^{(s l_i)} \Big]^{(j_p j_q) 1} \| (S_i L_i) J_i, (00) 0, J_i \rangle \Big|^2. (43)$$

[+] in which the second-quantized creation operator to be used should be the operator producing the 4-components Dirac spinor [27], i.e. $a_{n\kappa m}^{\dagger} |0\rangle = |n\kappa m\rangle$.

The annihilation operator in (43) acts between the ion and the remaining atom while the creation operator acts on a different subset between the continuum vacuum and the free electron. Using the decoupling formula [19, 26], the contributions of the different subspaces factorize:

$$\langle (S_a L_a) J_a, (s l_c) j_c, J \, || \, \left[\mathbf{a}^{\dagger (s l_c)} \times \mathbf{a}^{(s l_i)} \right]^{(j_p j_q)1} || \, (S_i L_i) J_i, (00)0, J_i \rangle$$

$$= (-1)^{J_a + j_c - J} [J, 1, J_i]^{\frac{1}{2}} \begin{Bmatrix} j_c & 0 & j_p \\ J_a & J_i & j_q \\ J & J_i & 1 \end{Bmatrix} \langle (s l_c) j_c \, || \, \mathbf{a}^{\dagger (s l_c) j_p} \, || \, (00)0 \rangle \, \langle (S_a L_a) J_a \, || \, \mathbf{a}^{(s l_i) j_q} \, || \, (S_i L_i) J_i \rangle$$

$$= (-1)^{J + J_i + 1} [J, 1]^{\frac{1}{2}} [j_c]^{-\frac{1}{2}} \delta(j_c, j_p) \begin{Bmatrix} j_q & J_a & J_i \\ J & 1 & j_c \end{Bmatrix}$$

$$\times \langle (s l_c) j_c \, || \, \mathbf{a}^{\dagger (s l_c) j_p} \, || \, (00)0 \rangle \, \langle (S_a L_a) J_a \, || \, \mathbf{a}^{(s l_i) j_q} \, || \, (S_i L_i) J_i \rangle \, . \tag{44}$$

The reduced matrix elements of the annihilation and creation operator are calculated by eliminating the J dependence as follows

$$\langle (S_a L_a) J_a \, || \, \mathbf{a}^{(s l_i) j_q} \, || \, (S_i L_i) J_i \rangle = [J_a, j_q, J_i]^{\frac{1}{2}} \begin{Bmatrix} S_a & L_a & J_a \\ S_i & L_i & J_i \\ s & l_i & j_q \end{Bmatrix} \langle S_a L_a \, || \, \mathbf{a}^{(s l_i)} \, || \, S_i L_i \rangle \tag{45}$$

and

$$\langle (s l_c) j_c \, || \, \mathbf{a}^{\dagger (s l_c) j_c} \, || \, (00)0 \rangle = [j_c] \begin{Bmatrix} s & l_c & j_c \\ 0 & 0 & 0 \\ s & l_c & j_c \end{Bmatrix} \langle s l_c \, || \, \mathbf{a}^{\dagger (s l_c)} \, || \, 00 \rangle$$

$$= [j_c]^{\frac{1}{2}} [l_c, s]^{-\frac{1}{2}} \langle s l_c \, || \, \mathbf{a}^{\dagger (s l_c)} \, || \, 00 \rangle \, \delta(s l_c j_c) \, , \tag{46}$$

Using equations (30) and (34), the contribution (43) to the partial cross section becomes (setting $N_i = N$):

$$\mathcal{D}^{l_c}(J_a, J_i) = \sum_{J j_c} \left| (-1)^{N + 1 + J + J_i + j_c + S_a - S_i + L_a - L_i} \sqrt{N/2} \, (S_a L_a, l_i | \} S_i L_i) \, [j_c, J_a, S_i, L_i, J, J_i]^{\frac{1}{2}} \right.$$

$$\left. \times \sum_{j_i} t(\epsilon s l_c, n_i s l_i) \, [j_i] \begin{Bmatrix} S_a & L_a & J_a \\ S_i & L_i & J_i \\ s & l_i & j_i \end{Bmatrix} \begin{Bmatrix} j_i & j_c & 1 \\ l_c & l_i & s \end{Bmatrix} \begin{Bmatrix} j_i & J_a & J_i \\ J & 1 & j_c \end{Bmatrix} \right|^2 \, . \tag{47}$$

Remembering that the one-electron matrix elements (20) are j_c and j_i independent, one finally obtains a quadruple summation

$$\mathcal{D}^{l_c}(J_a, J_i) = \frac{N}{2} \, |(S_a L_a, l_i | \} S_i L_i) \, |^2 \, [J_a, S_i, L_i, J_i] \sum_J [J] \, |t(\epsilon s l_c, n_i s l_i)|^2$$

$$\times \sum_{j_c} \sum_{j_i} \sum_{j_i'} [j_c, j_i, j_i'] \begin{Bmatrix} S_a & L_a & J_a \\ S_i & L_i & J_i \\ s & l_i & j_i \end{Bmatrix} \begin{Bmatrix} S_a & L_a & J_a \\ S_i & L_i & J_i \\ s & l_i & j_i' \end{Bmatrix}$$

$$\times \begin{Bmatrix} j_i & j_c & 1 \\ l_c & l_i & s \end{Bmatrix} \begin{Bmatrix} j_i' & j_c & 1 \\ l_c & l_i & s \end{Bmatrix} \begin{Bmatrix} j_c & J & J_a \\ J_i & j_i & 1 \end{Bmatrix} \begin{Bmatrix} j_c & J & J_a \\ J_i & j_i' & 1 \end{Bmatrix} \, . \tag{48}$$

Moving the summation symbol over j_c to the right and using equation (33)/sect.12.2 of Varshalovich *al.* [15] (see also the Appendix)

$$\sum_{j_c} [j_c] \begin{Bmatrix} j_i & 1 & j_c \\ l_c & s & l_i \end{Bmatrix} \begin{Bmatrix} l_c & s & j_c \\ j_i' & 1 & l_i \end{Bmatrix} \begin{Bmatrix} j_i' & 1 & j_c \\ J & J_a & J_i \end{Bmatrix} \begin{Bmatrix} J & J_a & j_c \\ j_i & 1 & J_i \end{Bmatrix}$$

$$= \sum_{j_c} [j_c] \begin{Bmatrix} j_i & 1 & j_c \\ s & l_i & j_i' \\ l_i & l_c & 1 \end{Bmatrix} \begin{Bmatrix} j_i & 1 & j_c \\ J_a & J_i & j_i' \\ J_i & J & 1 \end{Bmatrix} = \begin{Bmatrix} - & j_i & s & l_i \\ 1 & - & l_i & l_c \\ J & J_i & - & 1 \\ J_i & J_a & j_i' & - \end{Bmatrix}, \qquad (49)$$

the summation over j_c in (48) is incorporated into the 12j-symbol. A compact and elegant expression is obtained:

$$\mathcal{D}^{l_c}(J_a, J_i) = \frac{N}{2} |(S_a L_a, l_i|\} S_i L_i) |^2 [J_a, S_i, L_i, J_i] \sum_J [J] |t(\epsilon s l_c, n_i s l_i)|^2$$

$$\times \sum_{j_i} \sum_{j_i'} [j_i, j_i'] \begin{Bmatrix} S_a & L_a & J_a \\ S_i & L_i & J_i \\ s & l_i & j_i \end{Bmatrix} \begin{Bmatrix} S_a & L_a & J_a \\ S_i & L_i & J_i \\ s & l_i & j_i' \end{Bmatrix} \begin{Bmatrix} - & j_i & s & l_i \\ 1 & - & l_i & l_c \\ J & J_i & - & 1 \\ J_i & J_a & j_i' & - \end{Bmatrix} \text{(50)}$$

If one further assumes that the one-electron reduced matrix elements are J-independent, they can be moved to the left of the summation symbol over J to take advantage of the following identity

$$\sum_J [J] \begin{Bmatrix} - & j_i & s & l_i \\ 1 & - & l_i & l_c \\ J & J_i & - & 1 \\ J_i & J_a & j_i' & - \end{Bmatrix} = \delta(j_i, j_i') [l_i, j_i]^{-1} \delta(l_i s j_i) \delta(j_i J_a J_i) \delta(l_i l_c 1), \qquad (51)$$

that can be derived using the graphical approach [13, 14, 15]. The final result is

$$\mathcal{D}^{l_c}(J_a, J_i) = \frac{N}{2} (S_a L_a, l_i |\} S_i L_i)^2 [J_a, S_i, L_i, J_i]^{\frac{1}{2}} [l_i]^{-\frac{1}{2}}$$

$$\times |t(\epsilon s l_c, n_i s l_i)|^2 \sum_{j_i} [j_i] \begin{Bmatrix} S_a & L_a & J_a \\ S_i & L_i & J_i \\ s & l_i & j_i \end{Bmatrix}^2. \qquad (52)$$

Note that the same term-independent result can be obtained from (48), thanks to the $6j$ orthogonality relations,

$$\sum_J [J] \begin{Bmatrix} j_c & J & J_a \\ J_i & j_i & 1 \end{Bmatrix} \begin{Bmatrix} j_c & J & J_a \\ J_i & j_i' & 1 \end{Bmatrix} = \delta(j_i, j_i') [j_i]^{-1}, \qquad (53)$$

and

$$\sum_{j_c} [j_c] \begin{Bmatrix} j_i & j_c & 1 \\ l_c & l_i & s \end{Bmatrix}^2 = [l_i]^{-1}, \qquad (54)$$

that reduce the summations over J, j_c, j_i' and j_i to a single sum over j_i.

Inserting (52) in the partial cross section formula (13) and using the one-electron reduced matrix elements (20), one finds

$$\sigma^{TI}(J_a, J_i) = \frac{4\pi^2\omega}{3c} \sum_{l_c} [l_c] \begin{pmatrix} l_c & 1 & l_i \\ 0 & 0 & 0 \end{pmatrix}^2 (\,\epsilon l_c \,|\, r \,|\, n_i l_i\,)^2 \, [J_a, S_i, L_i] \tag{55}$$

$$\times \, N \, (\,S_a L_a, l_i \,|\} \, S_i L_i\,)^2 \sum_{j_i} [\,j_i\,] \begin{Bmatrix} S_a & L_a & J_a \\ s & l_i & j_i \\ S_i & L_i & J_i \end{Bmatrix}^2 .$$

Knowing the relation (6), one realizes that the term-independent cross section of Pan and Starace (10) is fully recovered. However this expression emerges naturally from the $(jj)J$-coupling analysis, without calling for the knowledge of the angular momentum relation (5).

5. Conclusion

We have shown that the "surprising" agreement raised recently by Blondel *et al* [1, 6] between the "standard" and the Cox-Engelking-Lineberger formulae when estimating the fine structure photodetachment relative intensities is understood from the important work of Pan and Starace [5]. The bridge between the two formalisms can be resumed through a rather simple and useful angular momentum relation that, to the knowledge of the authors, has never been published as such in its explicit form. More important, the present work, adopting the irreducible tensorial expression of second quantization operators, reproduces Pan and Starace's parametrization of the photodetachment cross section. It provides an elegant and natural way to link Pan and Starace's approach (including the "standard" formula) with the fractional parentage Cox-Engelking-Lineberger formula in the term-independent approximation. It unifies the two formalisms through a "simple" recoupling of the spherical tensorial second quantized form of the E1 transition operator, from $(SL)J$ to $(jj)J$.

Appendix A.

Analytically, the following equation holds:

$$\sum_X [X] \begin{Bmatrix} a & f & X \\ d & q & e \\ p & c & b \end{Bmatrix}^2 = \sum_Y [Y] \begin{Bmatrix} a & b & Y \\ c & d & p \end{Bmatrix}^2 \begin{Bmatrix} c & d & Y \\ e & f & q \end{Bmatrix}^2 \tag{A.1}$$

and is hereafter demonstrated graphically. The squared $9j$-symbols are joined to a $12j$ symbol by removing the sum, the momentum X and the factor $[X]$, and connecting the loose ends,

$$\sum_X [X] \begin{Bmatrix} a & f & X \\ d & q & e \\ p & c & b \end{Bmatrix}^2 = \sum_X [X] \quad\quad\quad = \quad\quad .$$

The two pairs of momenta (c, d) are cut and rejoined by a new momentum Y to obtain:

$$= \sum_Y [Y] \quad\quad\quad\quad .$$

These two diagrams are cut in the middle through three momenta to get four $6j$-symbols,

$$= \sum_Y [Y] \quad\quad\quad\quad\quad$$

$$= \sum_Y [Y] \begin{Bmatrix} a & b & Y \\ c & d & p \end{Bmatrix}^2 \begin{Bmatrix} c & d & Y \\ e & f & q \end{Bmatrix}^2 .$$

The identity A.1 between the squared $9j$-symbol and the two squared $6j$-symbols is obtained. An equivalent expression, if applied to another set of momenta, is

$$\sum_j [j] \begin{Bmatrix} j_4 & j_5 & j \\ j_6 & j_7 & j_8 \\ j_1 & j_2 & j_3 \end{Bmatrix}^2 = \sum_{j'} [j'] \begin{Bmatrix} j_4 & j_3 & j' \\ j_2 & j_6 & j_1 \end{Bmatrix}^2 \begin{Bmatrix} j_2 & j_6 & j' \\ j_8 & j_5 & j_7 \end{Bmatrix}^2 , \tag{A.2}$$

from which equation (5) is derived using the symmetry properties of $6j$ and $9j$ symbols.

Note that A.1 is a special case of equation (33)/sect.12.2 of Varshalovich *al.* [15]

$$\sum_X [X] \begin{Bmatrix} a & f & X \\ d & q & e \\ p & c & b \end{Bmatrix} \begin{Bmatrix} a & f & X \\ h & r & e \\ s & g & b \end{Bmatrix} \tag{A.3}$$

$$= \sum_Y [Y] \begin{Bmatrix} a & b & Y \\ c & d & p \end{Bmatrix} \begin{Bmatrix} c & d & Y \\ e & f & q \end{Bmatrix} \begin{Bmatrix} e & f & Y \\ g & h & r \end{Bmatrix} \begin{Bmatrix} g & h & X \\ a & b & s \end{Bmatrix}$$

$$= (-1)^{-p+q-r+s} \begin{Bmatrix} - & a & d & p \\ f & - & q & c \\ g & s & - & b \\ r & h & e & - \end{Bmatrix},$$

that becomes, for $h = d, s = p, r = q, g = c$

$$\sum_X [X] \begin{Bmatrix} a & f & X \\ d & q & e \\ p & c & b \end{Bmatrix}^2 = \sum_Y [Y] \begin{Bmatrix} a & b & Y \\ c & d & p \end{Bmatrix}^2 \begin{Bmatrix} c & d & Y \\ e & f & q \end{Bmatrix}^2$$

$$= \begin{Bmatrix} - & a & d & p \\ f & - & q & c \\ c & p & - & b \\ q & d & e & - \end{Bmatrix}.$$

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